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CALCULAT?/BI 20861 CALCULAT?/AB

L1 12 ((DNA#(10A)MELT?)(20A)CALCULAT?)/BI,AB

=> d l1 1-12 bib ab

L1 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2004 ACS ON STN
AN 2001:671712 CAPLUS
DN 136:320824
TI ***Calculating*** sequence-dependent ***melting***
stability of duplex ***DNA*** oligomers and multiplex sequence
analysis by graphs
AU Benight, Albert S.; Pancoska, Petr; Owczarzy, Richard;
Vallone, Peter M.; Nesetril, Jaroslav; Riccelli, Peter V.
CS Department of Chemistry, University of Illinois, Chicago, IL,
60607, USA
SO Methods in Enzymology (2001), 340(Drug-Nucleic Acid
Interactions), 165-192 CODEN: MENZAU; ISSN: 0076-6879
PB Academic Press
DT Journal; General Review
LA English
AB A review with refs. The anal. methods for characterizing DNA
sequence-dependent thermodyn. stability have been reviewed. A
set of n-n sequence stability parameters is presented. Examples
in which these values are used to calc. the thermodyn. stability of
short duplex DNA oligomers are presented. The problem of detg.
sets of isothermal sequences is addressed by representing DNA
sequences as graphs. Representing DNA sequences by a graph
descriptor with special math. properties minimizes the
computational difficulty of detg. the no. of DNA sequences with
identical predicted thermodyn. stability. This is achieved by
replacement of a whole set of sequences by a single
representative. Applications of this concept were demonstrated
for sequences assembled from individual bases and sequences
assembled from oligomeric blocks. (c) 2001 Academic Press.
RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR
THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:746334 CAPLUS
DN 130:105911

TI Comparison of experimental to ***MELTSIM***
calculated ***DNA*** ***melting*** of the (A+T) rich
Dictyostelium discoideum genome: denaturation maps distinguish
exons from introns

AU Marx, Kenneth A.; Assil, Iman Q.; Bizzaro, J. W.; Blake, R. D.
CS Department of Chemistry, University of Massachusetts, Lowell,
MA, 01854, USA

SO Journal of Biomolecular Structure & Dynamics (1998), 16(2),
329-339 CODEN: JBSDD6; ISSN: 0739-1102

PB Adenine Press

DT Journal

LA English

AB The slime mold, Dictyostelium discoideum, possesses an
(A+T) rich eukaryotic genome that is being sequenced in the
Human Genome Project. High resoln. melting curves of isolated
total and fractionated nuclear D. discoideum DNA (AX3 strain)
were detd. exptl. and are compared to melting curves calcd. from
GENBANK sequences (1.59% of genome) by the statistical
thermodn. program MELTSIM, parameterized for long DNA
sequences. The lower and upper temp. limits of calcd. melting
agree well with the obsd. melting of total DNA. The exptl. curve
is unusual in that it contains a no. of sharp peaks. MELTSIM
allowed us to calc. positional denaturation maps of D. discoideum
GENBANK sequence documents contg. the 26S, 5.8S and 17S
rDNA gene sequences, a major satellite DNA and repetitive
sequence family present in 100-200 copies/nucleus. These
denaturation maps contain subtransitions that correspond with a
no. of the exptl. obsd. peaks, some of which we show to
correspond with rDNA gene enriched CsCl gradient fractions of D.
discoideum DNA. MELTSIM calcd. curves of coding, intron and
flanking sequences indicate that both intron and flanking
sequences are extremely (A+T) rich and account for most of the
low temp. melting. There is no temp. overlap between thermal
stabilities of these sequence domains and those of coding DNA.
The latter must satisfy triplet codon constraints of higher (G+C)
content. These large stability property differences enable a
denaturation mapping feature of MELTSIM to clearly distinguish
exon positions from those of introns and flanking DNA in long D.
discoideum gene contg. sequences.

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR
THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:593023 CAPLUS
DN 129:299874

TI ***Melting*** of cross-linked ***DNA***. III.
Calculation of differential ***melting*** curves

AU Lando, Dmitri Y.; Fridman, Alexander S.; Krot, Vladimir I.;
Akhrem, Afanasii A.

CS Institute of Bioorganic Chemistry, Belarus National Academy
of Sciences, Minsk, 220141, Belarus

SO Journal of Biomolecular Structure & Dynamics (1998), 16(1),
59-67 CODEN: JBSDD6; ISSN: 0739-1102

PB Adenine Press

DT Journal

LA English

AB In our previous papers I and II (D. Y. Lando et al, J. Biomol.
Struct. Dynam. (1997) v. 15, N1, p.129-140, p. 141-150), two
methods were developed for calcn. of melting curves of cross-
linked DNA. One of them is based on Poland's and another on the
Fixman-Freire approach. In the present communication, III, a
new theor. method is developed for computation of differential
melting curves of DNAs cross-linked by anticancer drugs and their
inactive analogs. As Poland's approach, the method allows study

of the influence of the loop entropy factor, $\Delta(n)$, on melting
behavior (n is the length of a loop in base pairs). However the
method is much faster and requires computer time that inherent
for the most rapid Fixman-Freire calcn. approach. In contrast to
the computation procedures described before in communications
I and II, the method is suitable for computation of differential
melting curves in the case of long DNA chains, arbitrary loop
entropy factors of melted regions and arbitrary degree of
crosslinking including very low values that occur in vivo after
administration of antitumor drugs. The method is also
appropriate for DNAs without cross-links. The results of calcn.
demonstrate that even very low degree of crosslinking alters the
DNA differential melting curve. Crosslinking also markedly
strengthens the influence of particular function $\Delta(n)$ upon
melting behavior.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR
THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:142910 CAPLUS
DN 118:142910

TI Modified self-consistent phonon ***calculation*** of the
dependence of ***DNA*** ***melting*** temperature on
guanine-cytosine content

AU Feng, Y.; Tan, S. C.

CS Dep. Phys., Natl. Univ. Singapore, Singapore, 0511, Singapore
SO Physical Review A: Atomic, Molecular, and Optical Physics

(1992), 46(12), 8002-6 CODEN: PLRAAN; ISSN: 0556-2791

DT Journal

LA English

AB The self-consistent phonon approach was modified to treat
DNA double helixes modeled with a large repeating unit (N base
pairs) so that melting behaviors of DNA polymers of various base-
pair sequences can be studied. The melting temps. of DNA
polymers of different G-C-to-A-T ratios were calcd. (G, C, A, and
T denote guanine, cytosine, adenine, and thymine, resp.). A DNA
polymer with a relatively higher content of A-T melts at a lower
temp. than DNA with a higher content of G-C. The melting temp.
increases linearly when the G-C content in a DNA polymer
increases. This is in agreement with both exptl. observations and
theor. analyses.

L1 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:492436 CAPLUS
DN 111:92436

TI Long-range structural effects in supercoiled ***DNA*** :
statistical thermodynamics reveals a correlation between
calculated cooperative ***melting*** and contextual
influence on cruciform extrusion

AU Schaeffer, Francis; Yeramian, Edouard; Lilley, David M. J.
CS Dep. Biol. Mol., Inst. Pasteur, Paris, 75724, Fr.

SO Biopolymers (1989), 28(8), 1449-73 CODEN: BIPMAA; ISSN:
0006-3525

DT Journal

LA English

AB C-type inducing sequences, which cause cruciform extrusion
by adjacent inverted repeats were studied by applying statistical
thermodn. DNA helix melting theory. There was a marked
correlation between the ability of sequences to confer C-type
cruciform character exptl. and their calcd. propensity to undergo
cooperative melting, and no exceptions were found. The
correlations are both qual. and quant. Thus the ColE1 flanking
sequences behave as single melting units, whereas the DNA of
the S-type plasmid pIRbke8 exhibits no propensity to melt in the
region of the bke cruciform. The results of the calcns. are also
fully consistent with the following exptl. observations: (1) the
ability of the isolated colL and ColR fragments of the ColE1

flanking sequences, as well as the short sequence col30, to confer C-type character; (2) C-type induction by an adenine- and thymine-rich Drosophila sequence; (3) low-temp. cruciform extrusion by an (AT)₃₄ sequence; (4) the effect of changing sequences at a site 90 base pairs removed from the inverted repeat; (5) the effects of systematic deletion of the coll sequence; and (6) the effects of insertion of various sequences in between the coll sequence and the xke inverted repeat. Telestability effects on thermal denaturation as predicted from equil. helix melting theory of linear DNA may explain all the features that are revealed by studying the extrusion of cruciforms in circular DNA subjected to superhelical stress.

L1 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:149988 CAPLUS

DN 110:149988

TI ***Calculated*** ***melting*** temperature of methylated Z- ***DNA***

AU Hua, X.; Feng, Y.; Prohofsky, E. W.

CS Dep. Phys., Purdue Univ., Lafayette, IN, USA

SO Report (1988), Order No. AD-A193115, 22 pp. Avail.: NTIS From: Gov. Rep. Announce. Index (U. S.) 1988, 88(18), Abstr. No. 847,050

DT Report

LA English

AB There are 2 approaches to theor. calcn. of DNA melting temp. One is based on a 2 states, quasi-1-dimensional lattice model in which the melting profile and differentiated melting curve could be calcd. as a function of DNA length. Another way is the modified self-consistent effective phonon approxn. (MSPA) in which the dynamic motional behavior of the DNA mol. during the melting process is detailed. The later approach to melting of methylated Z-DNA was used and results were compared to a similar calcn. on unmethylated B-DNA. A calcn. of melting temp. of methylated Z-DNA based on MSPA was presented.

L1 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:420072 CAPLUS

DN 101:20072

TI ***Calculator*** -controlled high resolution ***melting*** measurements of bacterial ***DNAs***; basic information for taxonomy studies. (Proposal and reality)

AU Pivec, L.; Vitek, A.; Rozkot, F.; Formanek, P.; Tille, D.; Felsberg, J.; Prauser, H.

CS Inst. Mol. Genet., Czech. Acad. Sci., Prague, Czech.

SO Colloque INSERM (1983), 114(Baccilles Gram Negat. Interet Med. Sante Publique), 39-47 CODEN: CINMDE; ISSN: 0768-3154

DT Journal

LA English

AB The absorption melting profiles of DNAs from various bacterial species were detd. by using a spectrophotometer connected to a computer, and the melting curves were used for calcg. phylogenetic relations among bacteria by using various methods (e.g., the function distance and the genetic distance methods, and computer tomog.). DNA from each bacterial strain showed a specific melting profile. None of the methods used for detg. phylogenetic relations provided full correlation with DNA hybridization results (although the function distance method showed the best correlation). A single absorption melting curve did not provide sufficient information for the anal. of the melting substructure.

L1 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:599242 CAPLUS

DN 95:199242

TI Effect of selectively-binding ligands on ***DNA*** helix-coil transition. III. ***Calculation*** of the ***melting*** curve of ***DNA*** -ligand complexes

AU Akhrem, A. A.; Lando, D. Yu.

CS Inst. Bioorg. Chem., Minsk, USSR

SO Molekulyarnaya Biologiya (Moscow) (1981), 15(5), 1083-92

CODEN: MOBIBO; ISSN: 0026-8984

DT Journal

LA Russian

AB DNA with a low degree of heterogeneity (synthetic periodic heteropolynucleotides and satellite DNA) exhibited little change in the temp. interval of melting in the presence of increasing concns. of selectively (guanine-cytosine) and nonselectively binding destabilizing and stabilizing ligands. DNA with a high degree of heterogeneity (the major part of DNA of higher organisms) exhibited a broadening of the temp. interval of melting and an increase (or decrease) in the melting temp. in the presence of increasing concns. of selectively binding stabilizing (or destabilizing) ligands. Nonselectively binding ligands at increasing concns. had little effect on melting temp. and a modest effect on the temp. interval of melting. There is apparently a change in the adenine-thymine:guanine-cytosine ratio in helical and melted segments of high-heterogeneity DNA as denaturation proceeds, and the availability of new ligand binding sites results in broadening of the melting temp. range. This ratio does not change in DNA of low heterogeneity.

L1 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:204033 CAPLUS

DN 94:204033

TI Stabilities of nearest-neighbor doublets in double-helical

DNA determined by fitting ***calculated***

melting profiles to observed profiles

AU Gotoh, Osamu; Tagashira, Yusaku

CS Dep. Biochem., Saitama Cancer Cent. Res. Inst., Saitama, 362, Japan

SO Biopolymers (1981), 20(5), 1033-42 CODEN: BIPMAA; ISSN: 0006-3525

DT Journal

LA English

AB Melting profiles were calcd. for restriction fragments of .vphi.X174 and fd phage DNAs and compared with exptl. profiles. The algorithm of M. Fixman and J.J. Freire (1977) was slightly modified so that a stability parameter was assigned not to a base pair but to each nearest-neighbor doublet. Stabilities of the 10 kinds of nearest-neighbor doublets were estd. by fitting the calcd. profiles to the obsd. ones. Agreement of the calcd. and obsd. profiles was much improved by this modification. The most interesting finding was that purine (3'-5') pyrimidine stackings are much more stable than their resp. reverses. The order of nearest-neighbor stabilities is in excellent agreement with that of neg. stacking energies calcd. by R. Rein and coworkers (1973) by a quantum-chem. method.

L1 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:82692 CAPLUS

DN 86:82692

TI The disordered Ising chain: Equivalent formulations for the thermodynamics

AU Chalupa, J.; Grinstein, G.; Wortis, Michael

CS Dep. Phys., Univ. Illinois, Urbana, IL, USA

SO Journal of Chemical Physics (1976), 65(11), 4512-14 CODEN: JCPSA6; ISSN: 0021-9606

DT Journal

LA English

AB For a 1-dimensional spin-(1/2) Ising model in which the exchange constant between each neighboring pair of spins and

the magnetic field at each spin site are random variables, the free energy can be expressed in terms of the soln. to a homogeneous integral equation derived by A. A. Vedenov and A. M. Dykhne (1968) and C. Fan and B. M. McCoy (1969). In using this model to ***calculate*** the ***melting*** curve of ***DNA***, G. W. Lehman and J. P. McTague (1968) gave 2 equiv. inhomogeneous equations that determine the free energy. These formalisms are shown to be equiv. by transforming the homogeneous equation into the inhomogeneous equations. A formal representation of the free energy as an infinite continued fraction is given.

L1 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:503008 CAPLUS
DN 69:103008
TI ***Calculation*** of ***melting*** curves for ***DNA***
AU Crothers, Donald M.
CS Yale Univ., New Haven, CT, USA
SO Biopolymers (1968), 6(10), 1391-404 CODEN: BIPMAA; ISSN: 0006-3525
DT Journal
LA English
AB A method is reported for calcg. the melting curve of a DNA mol. of random base sequence, including in the calcns. the dependence of the free energy of base pair formation on the size of a denatured section. Particular attention is drawn to the variation of local melting behavior from one region of the mol. to another. Sections rich in AT melt at relatively low temps. with a fairly broad transition curve, whereas regions rich in GC pairs melt at higher temps. with a very abrupt local transition curve. To account qual. for the results, one may divide melting into two kinds of processes: (a) the nucleation and growth of denatured regions, and (b) the merging together of two denatured sections at the expense of the intervening helix. The first of these processes dominates in the first stages of melting, and leads to rather broad local melting curves. The second process predominates in the later stages, and occurs, in a particular part of the mol., over a very narrow temp. range. It is estd. that the av. length of a helix plus adjacent coil section at the midpoint of the transition is approx. 600 base pairs. Since transition curves which measure the local melting behavior reflect local compn. fluctuations, these curves contain information about the broad outlines of base sequence in the mol. Some suggestions are made concerning experiments by which this potential informations source could be exploited. Thus, one might map AT- or GC-rich regions at particular genetic loci in a biol. active DNA mol. Values of the relevant parameters found earlier for the transition of homopolymers produce melting curves for a DNA of random base sequence which are in good agreement with the exptl. transition curve for T2 phage DNA. Therefore, the present theoretical picture of the melting of polynucleotides is at least internally self-consistent.

L1 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:400092 CAPLUS
DN 69:92
TI A semiempirical analysis of the ***melting*** curves of synthetic ***DNA*** molecules and the ***calculation*** of the stacking and pairing energies and entropies in DNA
AU Goel, Narendra S.; Fukuda, Nobuo; Rein, Robert
CS Univ. of Rochester, Rochester, NY, USA
SO Journal of Theoretical Biology (1968), 18(3), 350-70 CODEN: JTBIAP; ISSN: 0022-5193
DT Journal
LA English
AB A semi-empirical anal. of the available exptl. data on the melting temps. and widths of the melting curves of various

synthetic DNAs was made using a modified Ising model with the nearest-neighbor interactions only, and values for the entropies of denaturation, A-T and G-C bonds energies, and stacking energies for the various nearest-neighbor base pairs were calcd. These values fell within a chem. reasonable range, suggesting that the modified Ising model with nearest-neighbor interactions only, is internally consistent, and satisfactorily describes the melting phenomenon. 30 references.

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